

Microwave spectrum and quadrupole coupling constants of 3-chloropyridine

A. CHATTERJEE AND D. K. GHOSH

Saha Institute of Nuclear Physics, Calcutta 700009

(Received 15 July 1974)

The microwave spectrum of 3-chloropyridine has been studied in the 22.0–25.5 GHz and in the 30.0–31.0 GHz frequency range. A large number of lines have been observed and many *Q* and *R* branch transitions of both *a* and *b* types have been assigned. The rotational constants and the quadrupole coupling constants for both Cl^{35} and Cl^{37} species of the molecule in their natural isotopic abundance have been evaluated and are listed in table 1.

Table 1

	Cl^{35}	Cl^{37}
<i>A</i>	5839.652 ± 0.015 MHz	5839.575 ± 0.024 MHz
<i>B</i>	1604.392 ± 0.007 ..	1558.825 ± 0.005 ..
<i>C</i>	1258.531 ± 0.007 ..	1230.299 ± 0.005 ..
<i>K</i>	-0.8490058	-0.8574502
<i>I_a</i>	86.5687 amu Å ²	86.5698 amu Å ²
<i>I_b</i>	315.0919 ..	324.3026 ..
<i>I_c</i>	401.6834 ..	410.9009 ..
$\Delta = (I_c - I_a - I_b)$	0.0228 ..	0.0285 ..
χ_{aa}	-71.58 ± 1.02 MHz	-57.35 ± 0.95 MHz
χ_{bb}	37.63 ± 1.45 ..	31.11 ± 1.34 ..
χ_{cc}	33.95 ± 1.02 ..	26.24 ± 0.95 ..

Conversion factor = 505531.1 MHz amu Å².

Details of this work will be communicated shortly. At the time of completion of this work we learnt that Sharma *et al** of the Tata Institute of Fundamental Research, Bombay have also completed their work on the Cl^{35} species of this molecule. The rotational constants and the quadrupolar coupling constants evaluated by them agree very nearly with those reported by us here.

The authors are grateful to Dr. A. C. Legon of the Department of Chemistry, University College, London for providing us with some rapid scans of the spectra recorded on a H.P. Microwave Spectrometer in the 26.5–40.0 GHz range as well as a slow scan in the 30.0–31.0 GHz range of frequency. The authors would also like to thank Prof. A. K. Saha for his interest in this work.

* Private communication.